



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:57 am BST

PDB ID : 6UJY  
Title : HIV-1 wild-type reverse transcriptase-DNA complex with (-)-3TC-TP  
Authors : Lansdon, E.B.  
Deposited on : 2019-10-03  
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

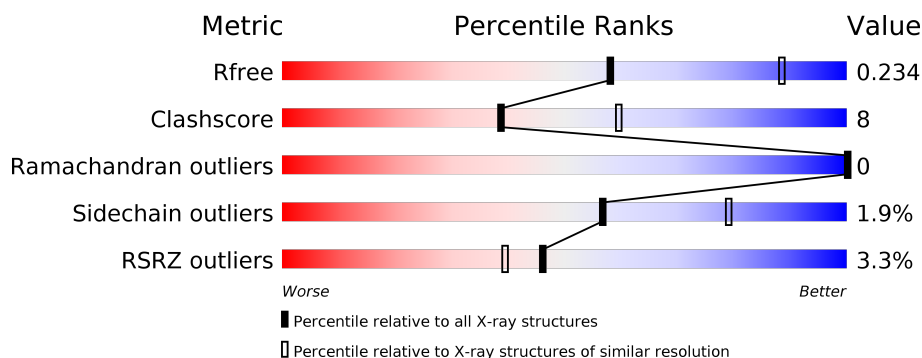
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	572	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	B	440	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
3	P	21	<div> <div></div> <div> <div></div> <div>71%</div> <div>14%</div> <div>14%</div> </div> </div>
4	T	27	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>30%</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8783 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called p66 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4471	2893	745	825	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04585
A	-10	GLY	-	expression tag	UNP P04585
A	-9	SER	-	expression tag	UNP P04585
A	-8	SER	-	expression tag	UNP P04585
A	-7	HIS	-	expression tag	UNP P04585
A	-6	HIS	-	expression tag	UNP P04585
A	-5	HIS	-	expression tag	UNP P04585
A	-4	HIS	-	expression tag	UNP P04585
A	-3	HIS	-	expression tag	UNP P04585
A	-2	HIS	-	expression tag	UNP P04585
A	-1	SER	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p51 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	391	Total	C	N	O	S	0	0	0
			3238	2104	537	591	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585

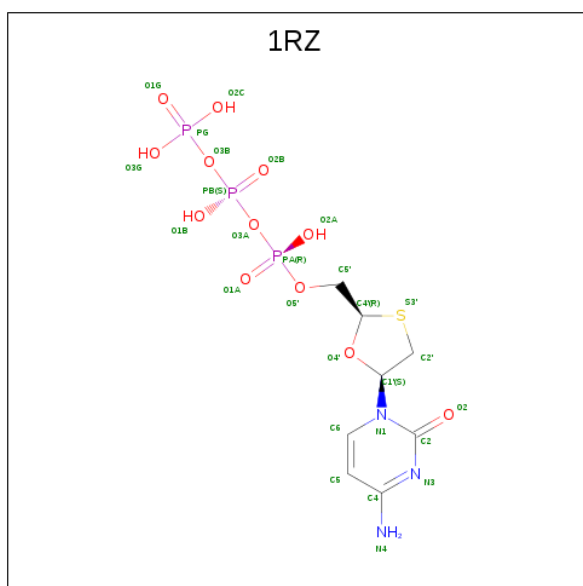
- Molecule 3 is a DNA chain called primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	P	0	0	0
			360	172	62	109	17			

- Molecule 4 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	22	Total	C	N	O	P	0	0	0
			460	214	95	129	22			

- Molecule 5 is Lamivudine Triphosphate (three-letter code: 1RZ) (formula:  $C_8H_{14}N_3O_{12}P_3S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	1
			54	16	6	24	6	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

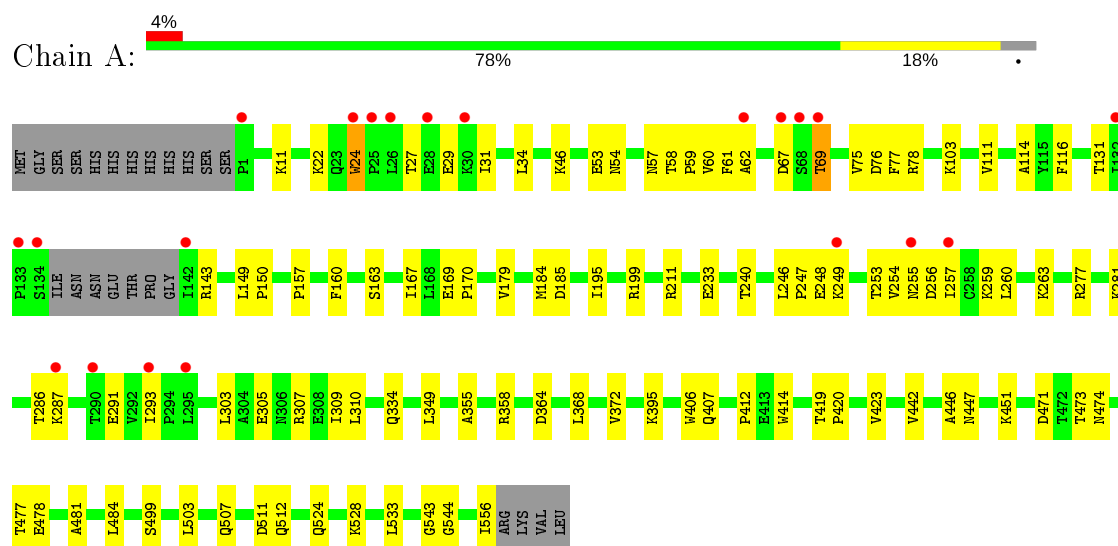
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total	O	0	0
			109	109		
8	B	54	Total	O	0	0
			54	54		
8	P	14	Total	O	0	0
			14	14		
8	T	12	Total	O	0	0
			12	12		

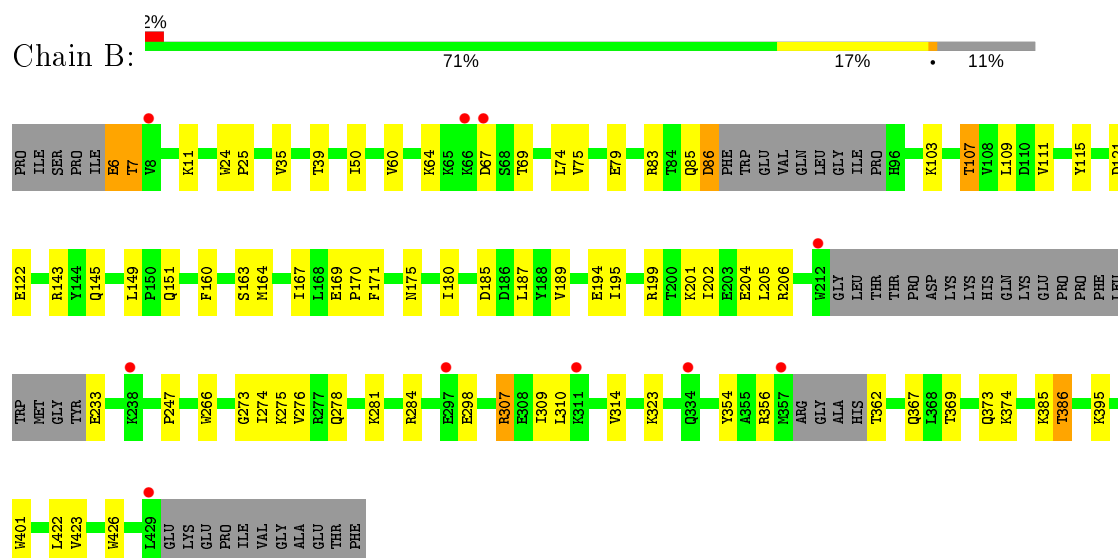
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: p66 Reverse transcriptase/RNaseH



- Molecule 2: p51 Reverse transcriptase/RNaseH



- Molecule 3: primer DNA





● Molecule 4: template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.70Å 169.48Å 102.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 2.59 47.46 – 2.59	Depositor EDS
% Data completeness (in resolution range)	80.5 (47.46-2.59) 85.1 (47.46-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.177 , 0.234 0.179 , 0.234	Depositor DCC
$R_{free}$ test set	2008 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, 1RZ, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.47	0/4586	0.58	0/6228
2	B	0.45	0/3325	0.61	0/4513
3	P	0.87	0/381	1.01	0/586
4	T	0.95	1/518 (0.2%)	0.88	1/799 (0.1%)
All	All	0.52	1/8810 (0.0%)	0.64	1/12126 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	706	DG	C3'-O3'	-6.21	1.35	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	707	DG	O4'-C4'-C3'	-5.40	102.34	104.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4471	0	4527	77	0
2	B	3238	0	3274	46	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	360	0	203	2	0
4	T	460	0	244	4	1
5	A	54	0	25	0	0
6	A	10	0	0	0	0
7	A	1	0	0	0	0
8	A	109	0	0	8	0
8	B	54	0	0	3	0
8	P	14	0	0	0	0
8	T	12	0	0	0	0
All	All	8783	0	8273	127	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:O	1:A:307:ARG:NH2	2.14	0.80
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.63	0.78
2:B:109:LEU:HD22	2:B:206:ARG:HD3	1.70	0.71
1:A:556:ILE:O	8:A:701:HOH:O	2.08	0.70
2:B:247:PRO:O	2:B:307:ARG:NH2	2.25	0.70
1:A:255:ASN:O	1:A:259:LYS:HG3	1.92	0.69
2:B:7:THR:HG21	2:B:121:ASP:HA	1.74	0.69
1:A:27:THR:HG22	1:A:29:GLU:H	1.58	0.67
1:A:277:ARG:NH1	1:A:334:GLN:O	2.28	0.66
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.78	0.66
2:B:122:GLU:OE2	8:B:501:HOH:O	2.14	0.65
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.78	0.65
2:B:163:SER:O	2:B:167:ILE:HG13	1.97	0.65
2:B:175:ASN:OD1	2:B:201:LYS:HE3	1.97	0.64
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.79	0.64
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.31	0.63
4:T:713:DC:H2'	4:T:714:DG:C8	2.33	0.63
1:A:54:ASN:O	1:A:143:ARG:NH2	2.28	0.62
1:A:447:ASN:HB2	1:A:556:ILE:HG23	1.81	0.61
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.66	0.60
1:A:53:GLU:CD	1:A:53:GLU:H	2.05	0.60
2:B:298:GLU:N	2:B:298:GLU:OE1	2.30	0.60
1:A:406:TRP:HZ3	1:A:507:GLN:HG2	1.65	0.60
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:A:355:ALA:O	2.35	0.60
1:A:233:GLU:OE1	8:A:703:HOH:O	2.17	0.59
1:A:131:THR:HG23	1:A:143:ARG:HG2	1.85	0.57
1:A:446:ALA:N	1:A:474:ASN:OD1	2.37	0.57
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.39	0.57
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.87	0.57
2:B:160:PHE:CE2	2:B:164:MET:HG2	2.39	0.57
3:P:816:DG:H2'	3:P:817:DG:C8	2.40	0.56
4:T:712:DC:H2'	4:T:713:DC:C6	2.39	0.56
2:B:199:ARG:NE	2:B:233:GLU:OE2	2.36	0.56
1:A:528:LYS:HE2	8:A:704:HOH:O	2.07	0.53
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.90	0.53
1:A:67:ASP:O	1:A:69:THR:OG1	2.26	0.53
1:A:407:GLN:NE2	8:A:707:HOH:O	2.42	0.52
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.91	0.52
1:A:287:LYS:HD2	1:A:291:GLU:OE2	2.09	0.52
2:B:386:THR:HG22	8:B:539:HOH:O	2.09	0.51
1:A:27:THR:HG22	1:A:29:GLU:N	2.24	0.51
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.93	0.51
1:A:157:PRO:HB3	1:A:184:MET:HE1	1.93	0.50
2:B:356:ARG:HG3	2:B:367:GLN:HG2	1.93	0.50
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.92	0.50
2:B:180:ILE:HD13	2:B:205:LEU:HD11	1.93	0.50
1:A:478:GLU:CG	1:A:499:SER:HB2	2.37	0.49
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.94	0.49
1:A:255:ASN:O	1:A:259:LYS:CG	2.59	0.49
2:B:278:GLN:O	2:B:281:LYS:HG2	2.13	0.49
2:B:35:VAL:O	2:B:39:THR:HG23	2.12	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.48	0.49
2:B:85:GLN:NE2	2:B:86:ASP:O	2.46	0.49
1:A:22:LYS:NZ	8:A:702:HOH:O	2.15	0.49
2:B:6:GLU:HG3	2:B:7:THR:N	2.28	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.95	0.48
2:B:281:LYS:HB2	2:B:284:ARG:NH1	2.28	0.48
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.96	0.48
1:A:524:GLN:OE1	8:A:704:HOH:O	2.19	0.48
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.95	0.48
1:A:195:ILE:O	1:A:199:ARG:HG3	2.14	0.48
1:A:478:GLU:HG3	8:A:714:HOH:O	2.14	0.47
1:A:24:TRP:HZ2	1:A:61:PHE:HD1	1.62	0.47
1:A:412:PRO:HD3	2:B:401:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.96	0.47
2:B:103:LYS:NZ	8:B:507:HOH:O	2.48	0.47
1:A:248:GLU:HG3	1:A:307:ARG:NH2	2.30	0.47
1:A:277:ARG:HH21	1:A:355:ALA:HB1	1.78	0.47
2:B:273:GLY:O	2:B:309:ILE:HD13	2.14	0.47
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.15	0.47
1:A:281:LYS:HE3	1:A:281:LYS:HB3	1.70	0.47
2:B:107:THR:HG21	2:B:202:ILE:HG13	1.97	0.46
1:A:286:THR:HB	1:A:291:GLU:OE1	2.15	0.46
2:B:171:PHE:HE1	2:B:204:GLU:HG2	1.81	0.46
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.98	0.46
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.80	0.46
2:B:79:GLU:HG3	2:B:83:ARG:NE	2.30	0.46
2:B:374:LYS:HD2	2:B:374:LYS:HA	1.75	0.46
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.97	0.45
1:A:478:GLU:HG2	1:A:499:SER:CB	2.39	0.45
2:B:143:ARG:HH11	2:B:143:ARG:HG2	1.81	0.45
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.82	0.45
1:A:406:TRP:CZ3	1:A:507:GLN:HG2	2.49	0.45
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.99	0.45
1:A:368:LEU:HD22	1:A:423:VAL:HG21	1.99	0.45
1:A:255:ASN:HD21	1:A:259:LYS:HD3	1.83	0.44
2:B:323:LYS:O	2:B:385:LYS:NZ	2.38	0.44
1:A:46:LYS:HE2	1:A:116:PHE:O	2.17	0.44
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.53	0.44
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.44
2:B:422:LEU:HD23	2:B:422:LEU:HA	1.76	0.44
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.53	0.44
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.75	0.43
1:A:503:LEU:HD12	1:A:533:LEU:HD23	2.00	0.43
1:A:211:ARG:NH1	8:A:711:HOH:O	2.50	0.43
2:B:395:LYS:HE3	3:P:813:DT:OP1	2.18	0.43
1:A:169:GLU:HB3	1:A:170:PRO:HD3	2.00	0.42
2:B:160:PHE:HE2	2:B:164:MET:HG2	1.82	0.42
2:B:11:LYS:HA	2:B:11:LYS:HD2	1.60	0.42
1:A:11:LYS:HB2	1:A:11:LYS:HE2	1.76	0.42
1:A:419:THR:HA	1:A:420:PRO:HD2	1.85	0.42
1:A:253:THR:O	1:A:257:ILE:HG12	2.20	0.42
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.19	0.42
1:A:305:GLU:O	1:A:309:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:724:DT:H2'	4:T:725:DG:O4'	2.19	0.42
1:A:259:LYS:O	1:A:263:LYS:HG2	2.19	0.42
2:B:64:LYS:NZ	2:B:69:THR:HA	2.35	0.42
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.41
1:A:484:LEU:HD12	1:A:484:LEU:HA	1.74	0.41
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.31	0.41
1:A:249:LYS:HZ3	1:A:256:ASP:CG	2.24	0.41
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.50	0.41
1:A:372:VAL:HG11	1:A:412:PRO:HD2	2.03	0.41
2:B:24:TRP:HB2	2:B:25:PRO:HD2	2.03	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.72	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.20	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.92	0.41
1:A:249:LYS:HZ2	1:A:256:ASP:HB3	1.85	0.41
2:B:180:ILE:HG23	2:B:189:VAL:HG22	2.02	0.40
1:A:543:GLY:HA2	1:A:544:GLY:HA2	1.64	0.40
2:B:354:TYR:OH	2:B:356:ARG:NE	2.54	0.40
1:A:24:TRP:HZ2	1:A:61:PHE:CD1	2.38	0.40
4:T:711:DC:H2'	4:T:712:DC:C6	2.56	0.40
2:B:201:LYS:O	2:B:204:GLU:HB3	2.21	0.40
1:A:303:LEU:HD21	1:A:307:ARG:NH1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:O	4:T:725:DG:N2[3_554]	2.08	0.12

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/572 (95%)	518 (95%)	27 (5%)	0	100	100
2	B	383/440 (87%)	371 (97%)	12 (3%)	0	100	100
All	All	928/1012 (92%)	889 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/511 (96%)	487 (99%)	3 (1%)	86	95
2	B	358/400 (90%)	345 (96%)	13 (4%)	35	61
All	All	848/911 (93%)	832 (98%)	16 (2%)	57	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	69	THR
1	A	240	THR
2	B	6	GLU
2	B	7	THR
2	B	67	ASP
2	B	74	LEU
2	B	86	ASP
2	B	107	THR
2	B	194	GLU
2	B	195	ILE
2	B	275	LYS
2	B	276	VAL
2	B	307	ARG
2	B	362	THR
2	B	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DOC	P	822	3,4	14,19,20	2.35	7 (50%)	13,26,29	4.28	6 (46%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOC	P	822	3,4	-	1/4/18/19	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C4-N3	4.85	1.43	1.35
3	P	822	DOC	O4'-C1'	3.23	1.49	1.42
3	P	822	DOC	C5-C4	-3.19	1.33	1.41
3	P	822	DOC	O5'-C5'	-2.77	1.38	1.44
3	P	822	DOC	C4-N4	2.68	1.43	1.35
3	P	822	DOC	C3'-C2'	-2.25	1.47	1.54
3	P	822	DOC	C6-N1	2.05	1.38	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	11.83	134.75	112.48
3	P	822	DOC	O4'-C4'-C5'	5.94	119.28	109.52
3	P	822	DOC	C2-N3-C4	4.29	120.69	116.34
3	P	822	DOC	C4'-O4'-C1'	-3.99	106.04	109.81
3	P	822	DOC	O4'-C1'-C2'	-3.91	102.43	106.67
3	P	822	DOC	O4'-C4'-C3'	2.07	108.24	104.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	822	DOC	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	SO4	A	602	-	4,4,4	0.19	0	6,6,6	0.20	0
6	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.15	0
5	1RZ	A	601[B]	7	22,28,28	0.89	0	27,43,43	1.63	5 (18%)
5	1RZ	A	601[A]	7	22,28,28	0.91	0	27,43,43	1.55	4 (14%)



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1RZ	A	601[B]	7	-	4/19/31/31	0/2/2/2
5	1RZ	A	601[A]	7	-	7/19/31/31	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601[A]	1RZ	C2-N3-C4	4.96	121.36	116.34
5	A	601[B]	1RZ	C2-N3-C4	4.95	121.36	116.34
5	A	601[B]	1RZ	PA-O3A-PB	-2.81	123.19	132.83
5	A	601[B]	1RZ	PB-O3B-PG	-2.52	124.19	132.83
5	A	601[B]	1RZ	O1B-PB-O2B	2.48	124.52	112.24
5	A	601[A]	1RZ	PB-O3B-PG	-2.38	124.65	132.83
5	A	601[B]	1RZ	O4'-C4'-C5'	-2.28	103.62	109.56
5	A	601[A]	1RZ	O4'-C4'-C5'	-2.16	103.92	109.56
5	A	601[A]	1RZ	O1B-PB-O2B	2.00	122.14	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

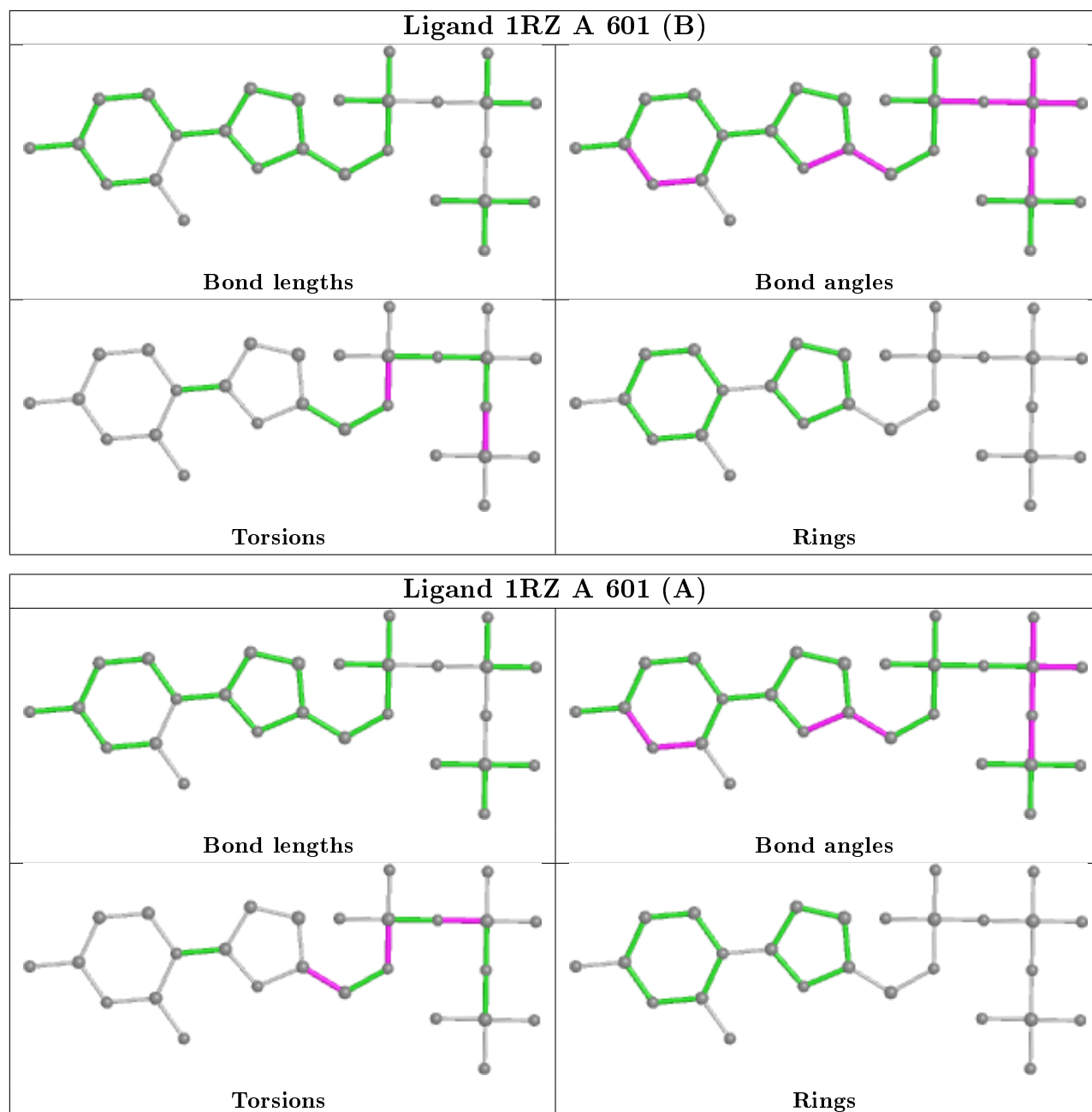
Mol	Chain	Res	Type	Atoms
5	A	601[B]	1RZ	PB-O3B-PG-O2C
5	A	601[B]	1RZ	C5'-O5'-PA-O3A
5	A	601[B]	1RZ	C5'-O5'-PA-O1A
5	A	601[A]	1RZ	C5'-O5'-PA-O3A
5	A	601[A]	1RZ	C5'-O5'-PA-O1A
5	A	601[A]	1RZ	C5'-O5'-PA-O2A
5	A	601[A]	1RZ	S3'-C4'-C5'-O5'
5	A	601[A]	1RZ	PA-O3A-PB-O2B
5	A	601[B]	1RZ	C5'-O5'-PA-O2A
5	A	601[A]	1RZ	PA-O3A-PB-O1B
5	A	601[A]	1RZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	549/572 (95%)	-0.01	21 (3%) 40 33	24, 42, 76, 108	0
2	B	391/440 (88%)	0.05	10 (2%) 56 50	24, 49, 78, 103	0
3	P	17/21 (80%)	-0.77	0 100 100	33, 51, 65, 67	0
4	T	22/27 (81%)	-0.32	1 (4%) 33 26	32, 61, 91, 104	0
All	All	979/1060 (92%)	-0.01	32 (3%) 46 39	24, 45, 78, 108	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	311	LYS	4.6
1	A	69	THR	4.5
1	A	26	LEU	4.4
2	B	212	TRP	4.2
1	A	68	SER	4.0
2	B	429	LEU	3.6
1	A	24	TRP	3.6
2	B	67	ASP	3.3
2	B	357	MET	3.1
1	A	67	ASP	2.9
1	A	287	LYS	2.8
1	A	133	PRO	2.8
2	B	66	LYS	2.7
1	A	62	ALA	2.7
1	A	134	SER	2.7
1	A	30	LYS	2.6
1	A	132	ILE	2.6
1	A	290	THR	2.5
2	B	238	LYS	2.5
2	B	334	GLN	2.5
1	A	257	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.3
1	A	25	PRO	2.3
1	A	1	PRO	2.3
1	A	142	ILE	2.2
2	B	297	GLU	2.2
1	A	249	LYS	2.1
1	A	255	ASN	2.1
1	A	28	GLU	2.1
1	A	295	LEU	2.1
4	T	704	DG	2.1
2	B	8	VAL	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DOC	P	822	18/19	0.99	0.14	27,32,41,42	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

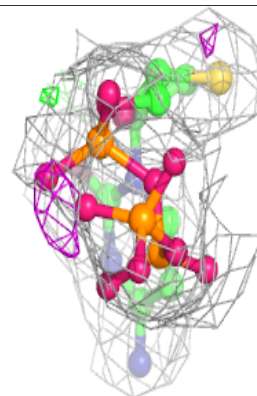
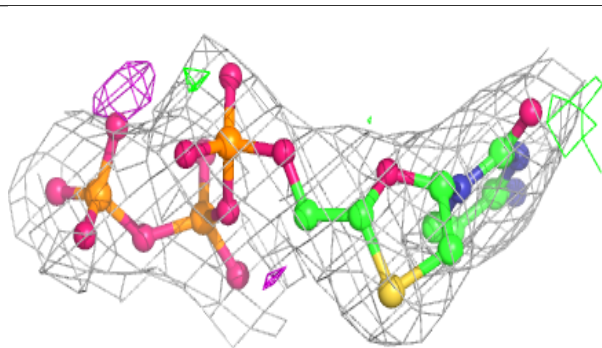
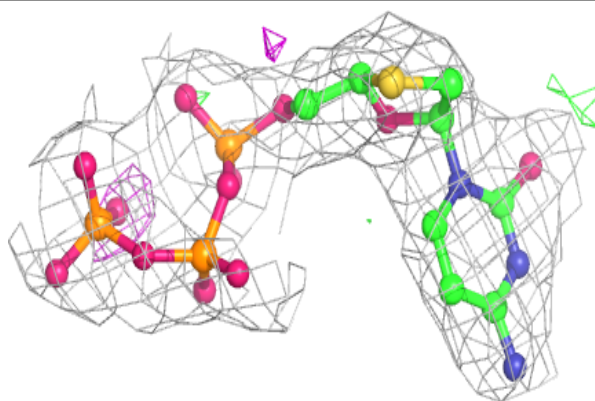
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	1RZ	A	601[B]	27/27	0.95	0.15	38,46,60,63	27
5	1RZ	A	601[A]	27/27	0.95	0.15	37,48,60,61	27
7	MG	A	604	1/1	0.96	0.11	45,45,45,45	0
6	SO4	A	603	5/5	0.97	0.07	68,71,81,87	0
6	SO4	A	602	5/5	0.98	0.10	42,50,57,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

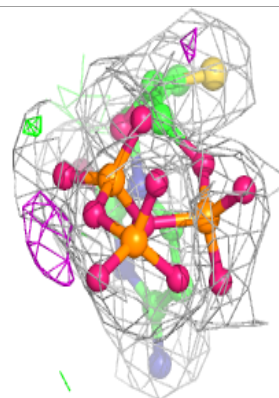
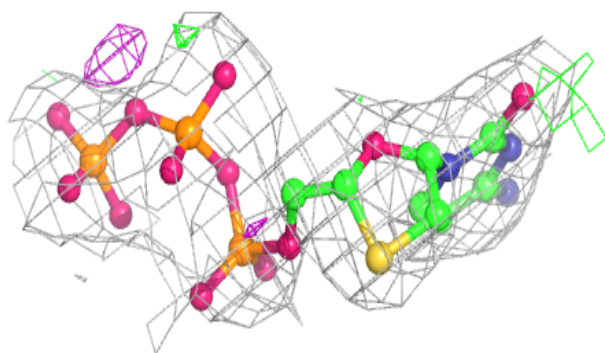
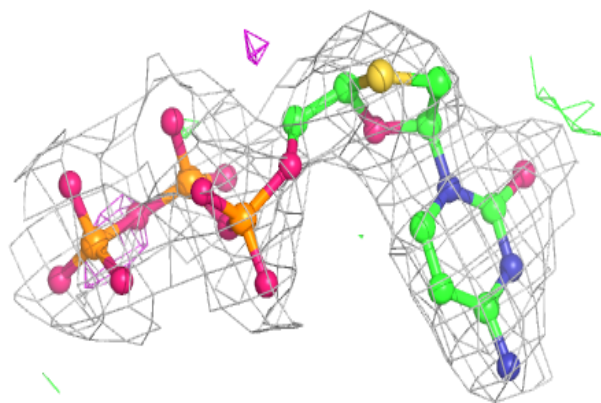
**Electron density around 1RZ A 601 (B):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 1RZ A 601 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.